# Towards Breaking Temperature Equilibrium in Multi-Component Eulerian Schemes

11th International Workshop on the Physics of Compressible Turbulent Mixing (IWPCTM11)
La Fonda Hotel, Santa Fe NM
July 14-18, 2008

John W. Grove**
Thomas Masser
*Computational Physics and Mathematics Group*
*Computer, Computational and Statistical Sciences Division*
*Los Alamos National Laboratory*

**Contact Email: jgrove@lanl.gov.





LA-UR-08-04758

# Acknowledgements


- Thomas Masser
  - Ph.D. student from Stony Brook
  - Thomas's work on a computational analysis of the effect of thermal equilibrium across material interfaces has help guide the selection and analysis of the multi-temperature cell models implemented here
- Mark Christon and Robert Lowrie
  - For many helpful discussions on multi-temperature flow models and their numerical implementation
  - Jointly helped formulate the numerical schemes implemented here


The cover is taken from computational comparisons of a strong shock implosion between RAGE and the front tracking code FronTier. FronTier maintains sharp interfaces and avoids mixed cells. It fully resolves the microstructure assumed by the following flow models. The colors represent temperature and illustrate the large hot spot temperatures that can be produced by shock heating of a dense material on a light material. This computation is part of the Ph.D. work of T. Masser.

# Algorithmic Differences/Similarities

- XRAGE/FronTier are both rectangular cell based codes with a finite volume Godunov scheme update.
- XRAGE – Pressure–Temperature equilibrium equation of state:
  - Conservation of total mass, momentum, and energy
  - Advection of mass fraction

$$\frac{\partial r}{\partial t} + -\sum\left(r\,\mathbf{u}\right) = 0$$

$$\frac{\partial r\,\mathbf{u}}{\partial t} + -\sum\left(r\,\mathbf{u}\,f\ \mathbf{u}\right) + -P = 0$$

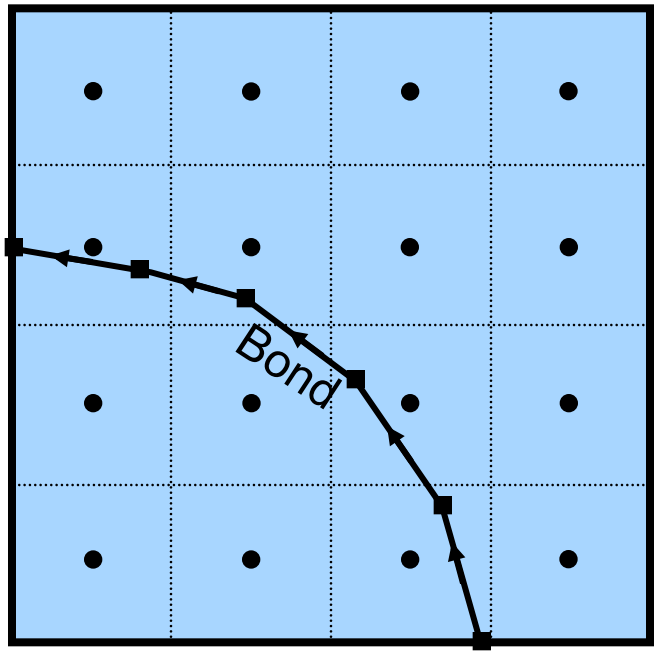
$$\frac{\partial r\left(\frac{1}{2}u^2 + e\right)}{\partial t} + -\sum\left(r\,\mathbf{u}\left(\frac{1}{2}u^2 + e\right)\right) + -\sum\left(P\mathbf{u}\right) = 0$$

$$a_k r_k = m_k r$$

$$\frac{Dm_k}{Dt} = \frac{\partial m_k}{\partial t} + \mathbf{u}\sum -m_k = 0$$

# Geometric Front Tracking

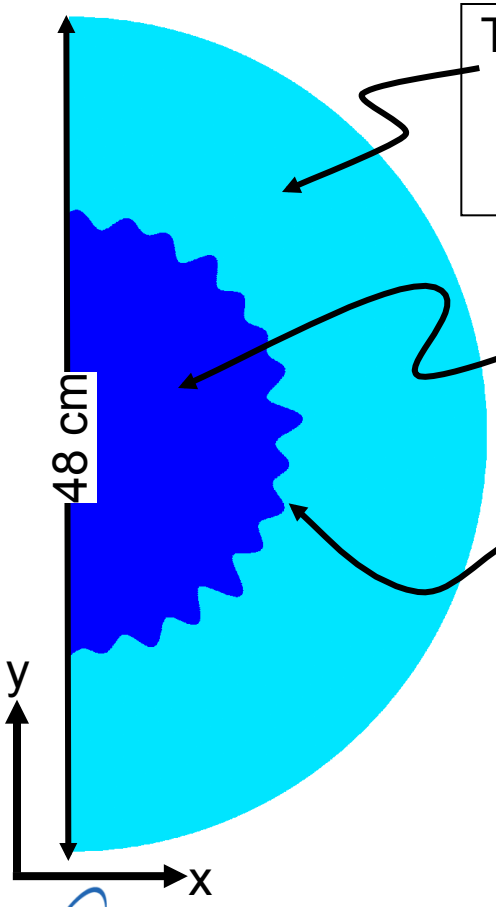
- Selected wave fronts are **explicitly** included in the discretization.
- The flow state consists of a composite grid with a spatial mesh overlaid with a co-dimension one mesh that **tracks** the fronts.
- The time stepping algorithm adapts to the local geometry of the front and fully couples interface motion with the the spatial mesh.
- In contrast to VOF methods the interface is preserved throughout the computation
  - Interface is propagated not reconstructed
  - Separates materials for EOS treatment, no mixed cells.
- The interface is propagated using Riemann problem solutions and method of characteristic approximations.
  - Interactions are treated explicitly.




- Grid State
- Tracked Points (left,right) States

# Cylindrical Implosion Test Problem Setup

Boundary Condition: ρ = 11.233 gram/cc, P = 0.686 Mbar, **v** = 0




Tin: ρ = 7.282 gram/cc, P = 1 bar, **v** = 0

$$\Gamma = 2.27, \mathrm{P}_{\infty} = 0.15 \text{ Mbar}, \mathrm{e}_{\infty} = 1.25 \times 10^{-8} \text{ 0.1 megajoules / gram}$$

$$\rho_0 = 7.287 \text{ gram / cc}, \mathrm{C}_{\mathrm{V}} = 2.2 \times 10^{-6} \text{ 0.1 megajoules / gram /}^{\circ} \text{ K}, \eta = 0.027$$

Air: ρ = 0.001047 gram/cc, P = 1 bar, **v** = 0

$$\Gamma = 0.402, P_{\infty} = 0 \text{ Mbar}, \ e_{\infty} = 0 \text{ 0.1 megajoules/gram}$$

$$\rho_0 = 0.001047 \text{ gram/cc}, \mathrm{C}_{\mathrm{V}} = 7.1368 \times 10^{-6} \text{ 0.1 megajoules/gram/}^{\circ}K, \eta = 0$$

Interface: $r = r_0 + \sum_{k=1}^{9} a_k \sin\left(\upsilon_k \left(\theta + \frac{\pi}{2}\right) + \phi_k\right)$

$\mathbf{a} = (0.208057, 0.017559, -0.0700731, -0.104933, -0.188979, 0.051327, -0.155088, -0.47643, 0.140691)$

$\boldsymbol{\upsilon} = (16, 18, 20, 22, 24, 26, 28, 30, 32)$

$\boldsymbol{\phi} = (0.945557, 4.56071, 4.85797, 6.13974, 3.09001, 4.84, 0.443656, 5.76627, 5.69294)$

EOS: Stiffened Gamma Law

$$P + \left(\Gamma + 1\right) P_{\infty} = \Gamma \left(e + e_{\infty}\right) \rho$$

$$e + e_{\infty} = C_V T + \frac{P_{\infty}}{\rho} + \eta \left(\frac{P_{\infty}}{\rho_0}\right) \left(\frac{\rho}{\rho_0}\right)^{\Gamma}$$

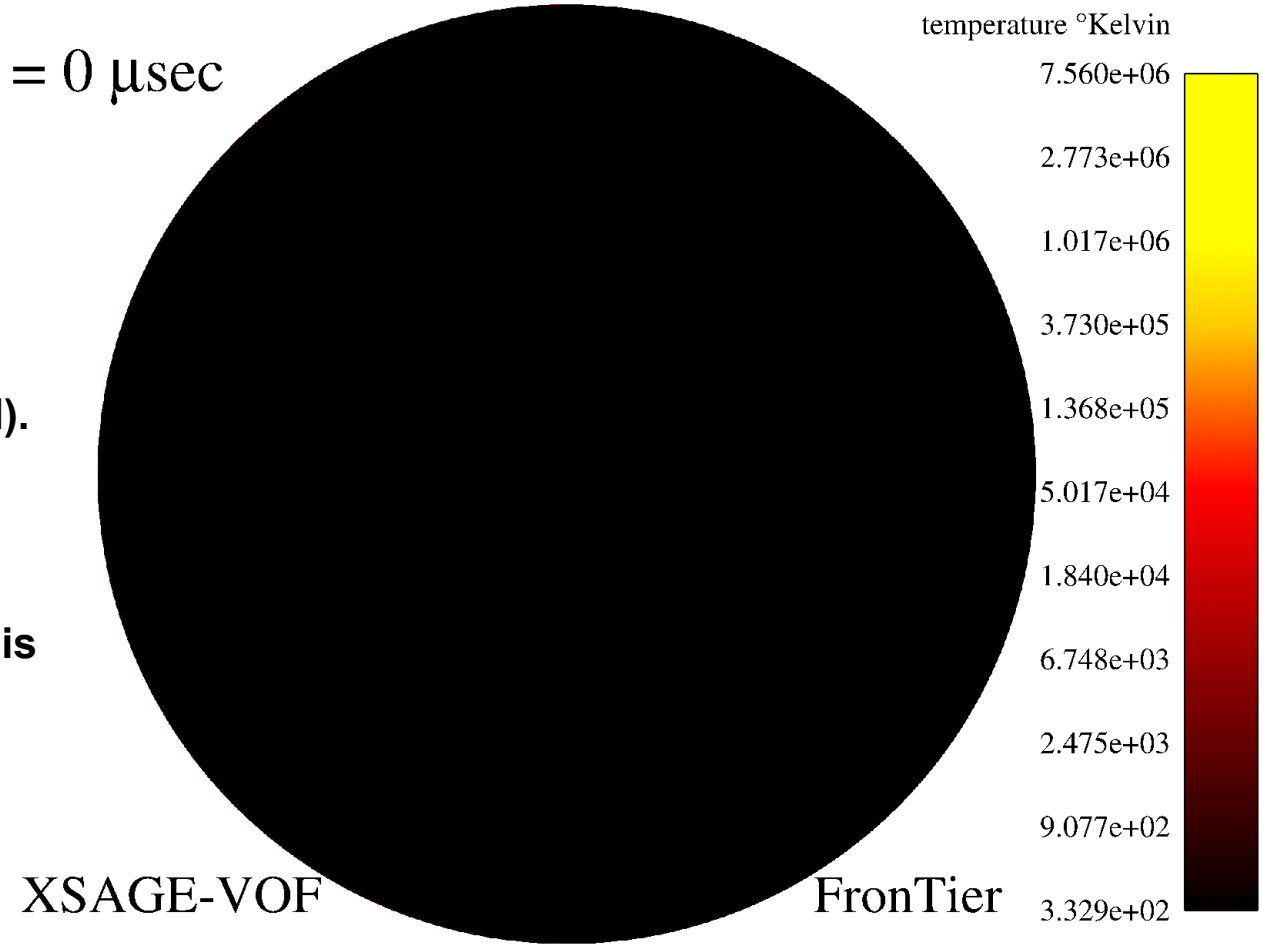
Los Alamos NATIONAL LABORATORY EST. 1943





LA-UR-08-04758

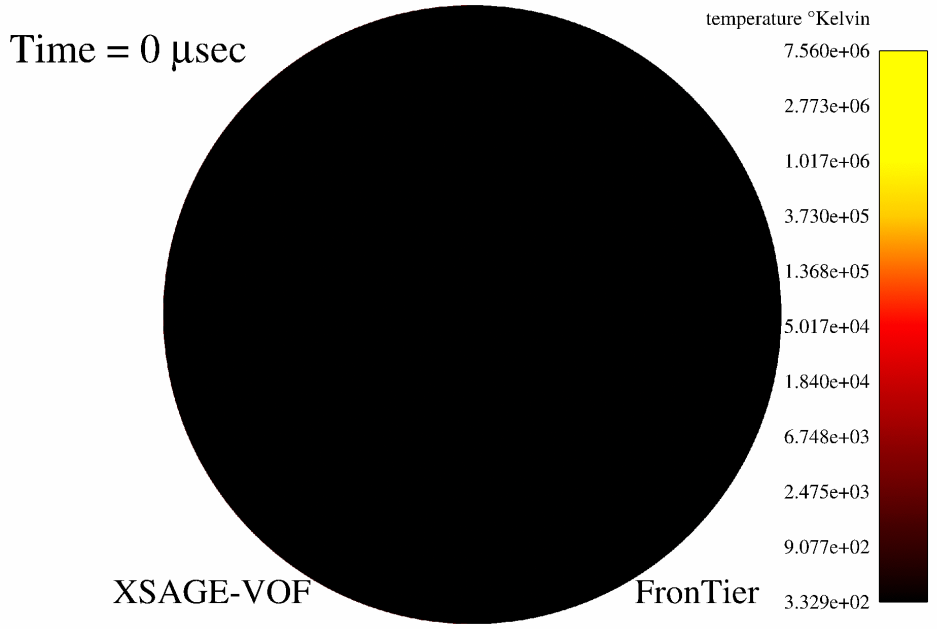
# Temperature

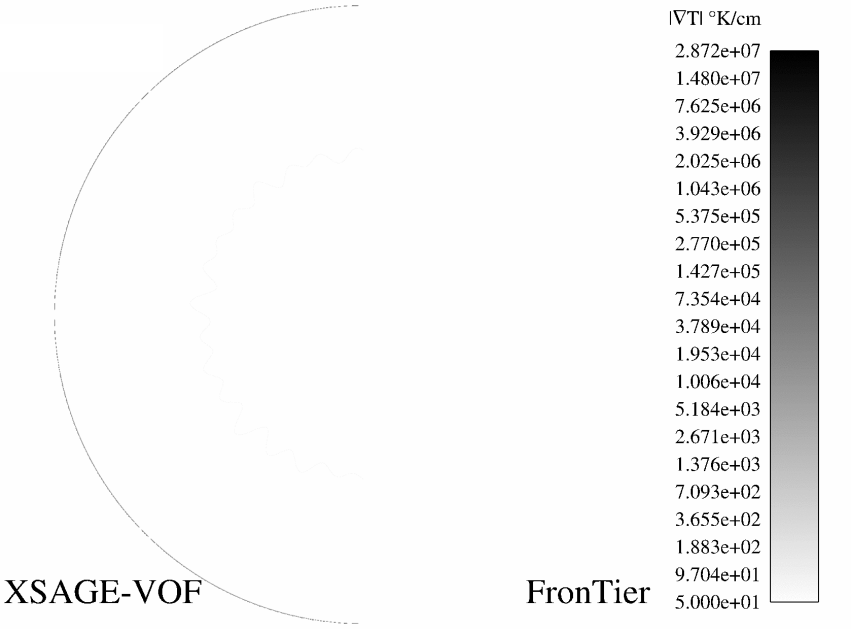



- **Shock heating of air in an order of magnitude higher when computed by FronTier (no T equilibrium imposed).**
- **Prior to reshock/ implosion the temperature jump across the interface is similar.**
- **FronTier produces a noticeably stronger reflected shock at implosion.**

# Temperature

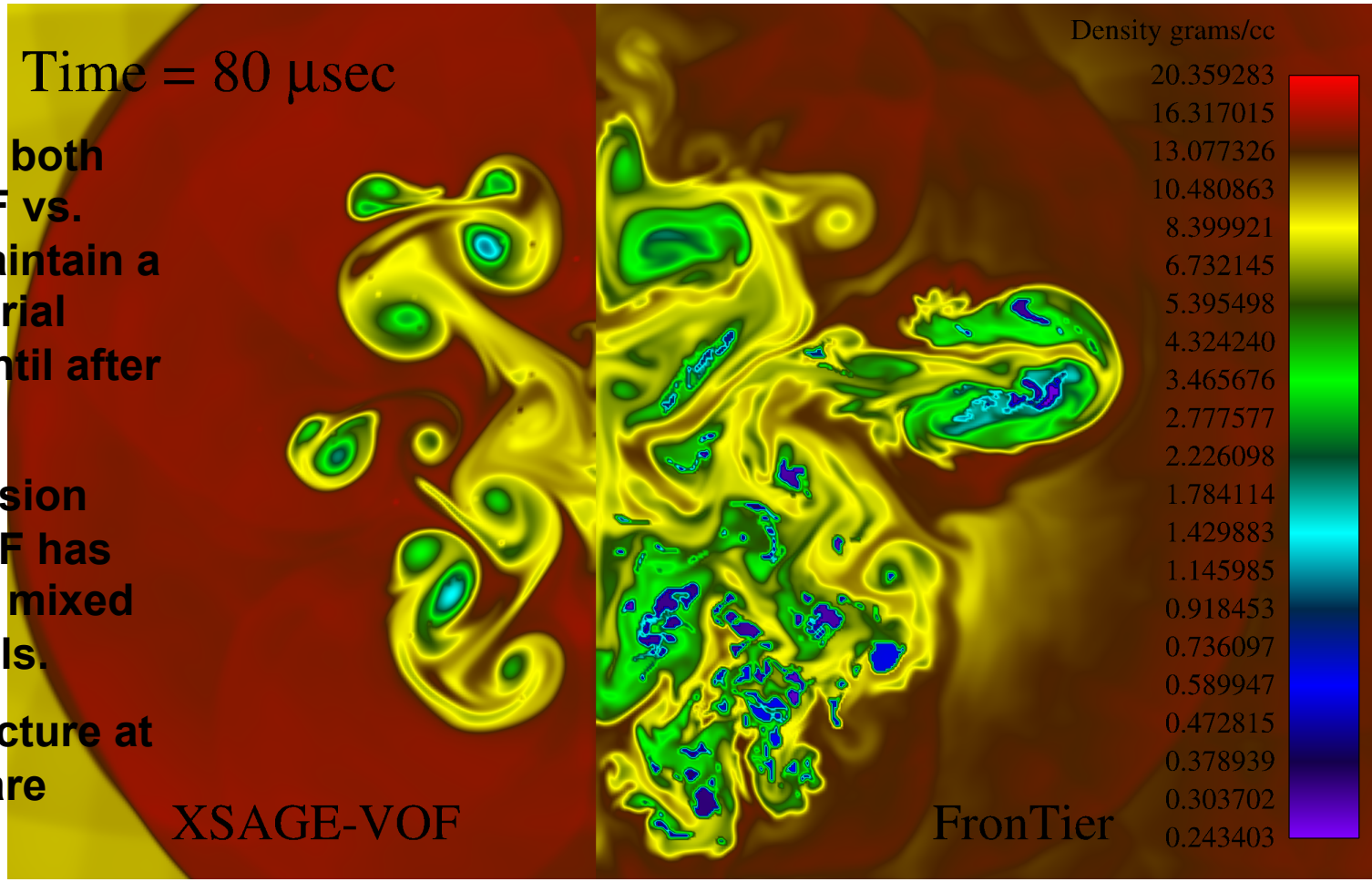
- Shock heating of air in an order of magnitude higher when computed by FronTier (no T equilibrium imposed).
- Prior to reshock/implosion the temperature jump across the interface is similar.
- FronTier produces a noticeably stronger reflected shock at implosion.



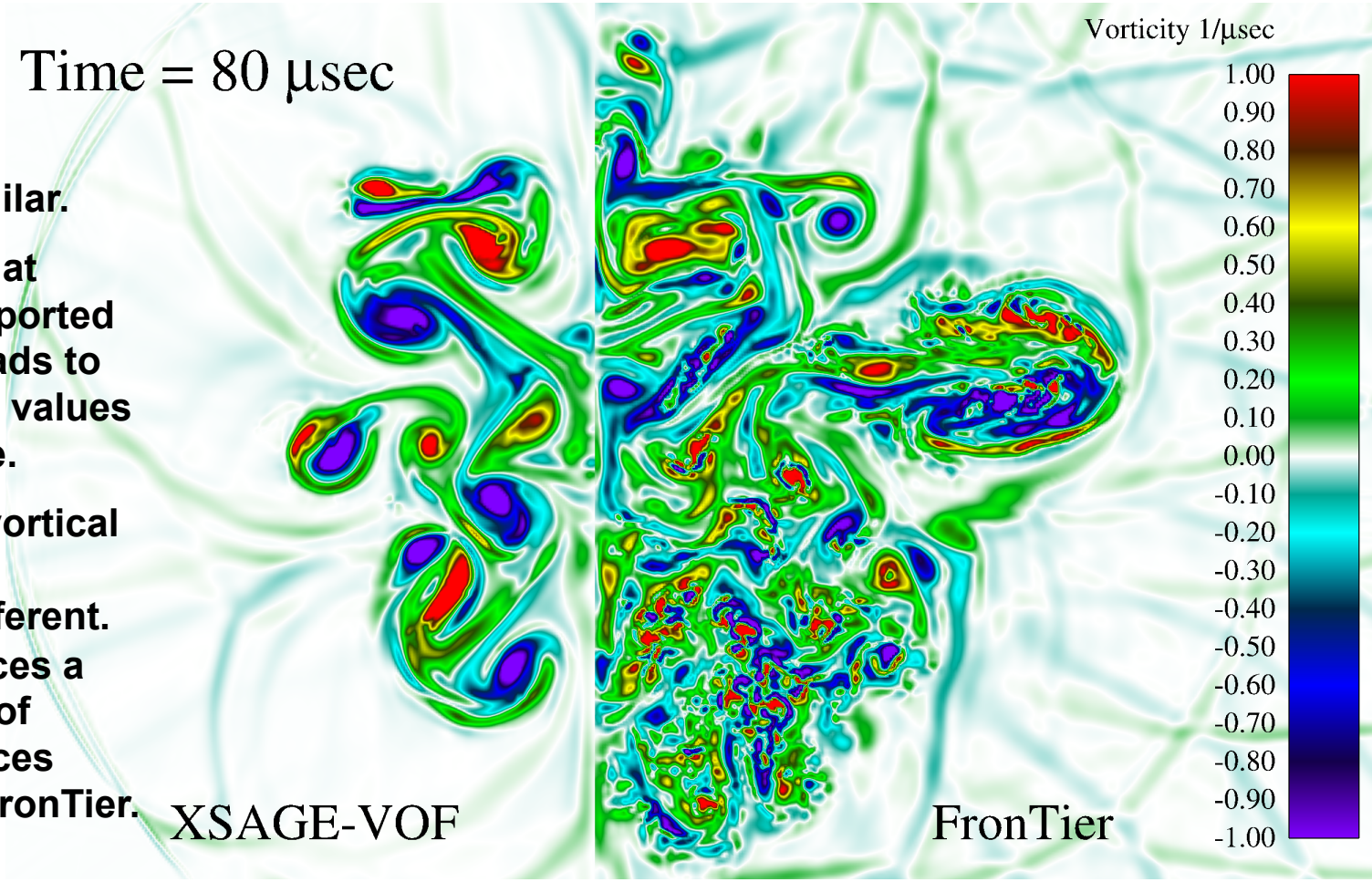
# Mass Density

- Tracking in both codes (VOF vs. explicit) maintain a sharp material interface until after implosion.
- After implosion XSAGE-VOF has completely mixed the materials.
- Vortex structure at late times are different.



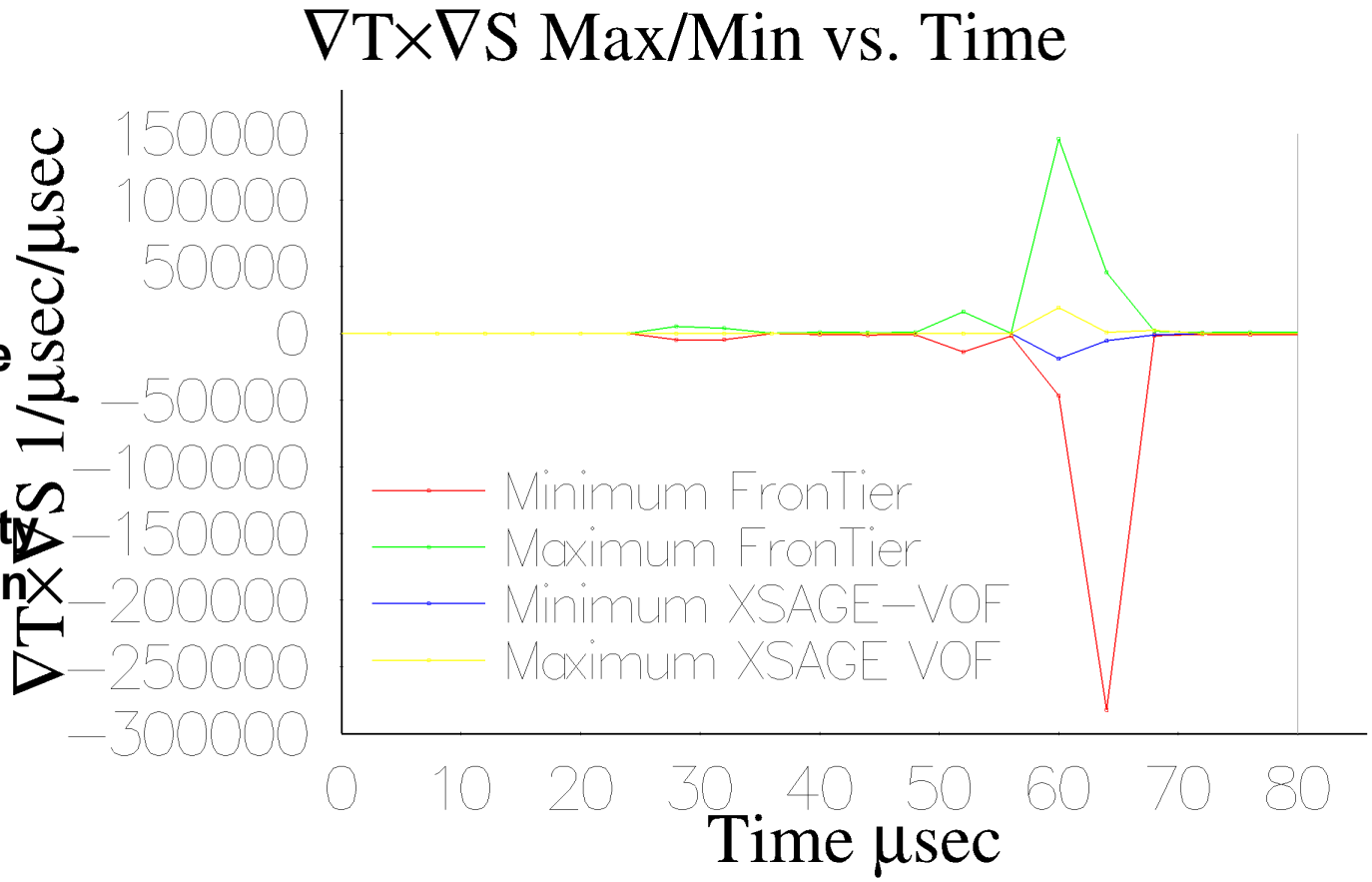
# Vorticity: Ñ´u

- **Pre-implosion vorticity is similar.**
- **Velocity shear at interfaces supported by FronTier leads to larger vorticity values at the interface.**
- **Late time the vortical structure is completely different. XSAGE produces a small number of coherent vortices compared to FronTier.**

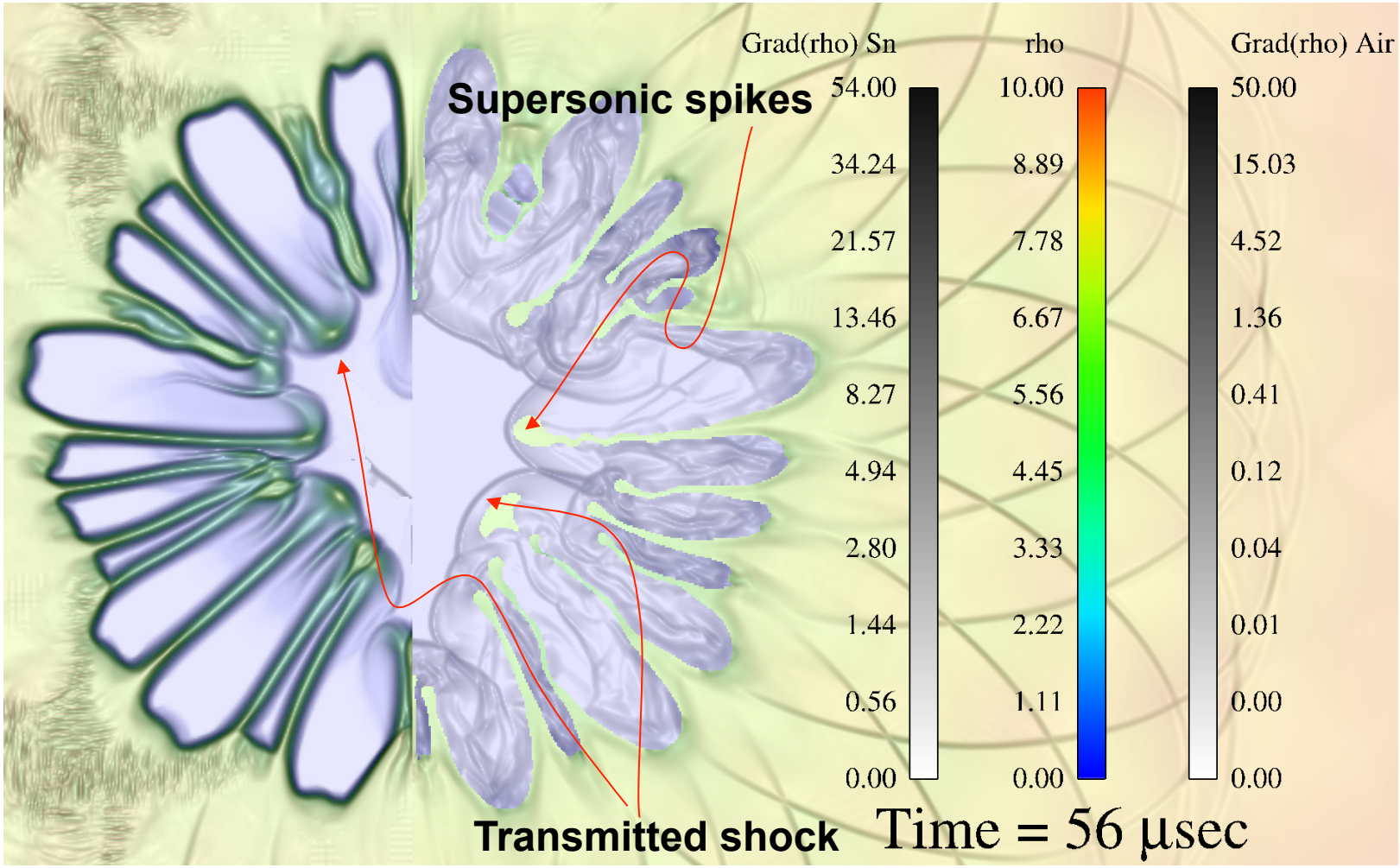


# Baroclinic Vorticity Source Term, ÑT´ÑS

- Vorticity sources are concentrated on interfaces.
- FronTier tracking together with large temperature gradients result in much large vorticity sources near air/Sn interfaces.

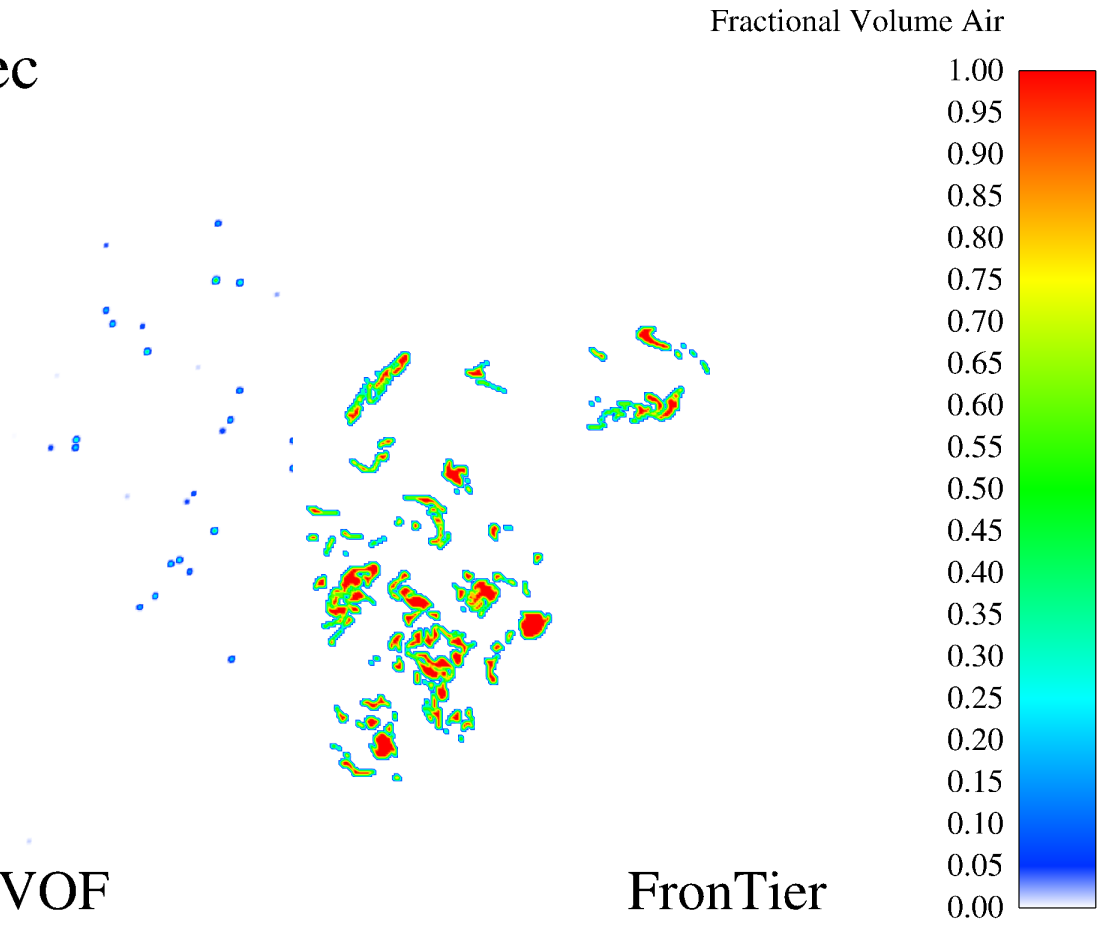


# Blowup of Composite Image Showing Bow Shocks



# Volume Fraction of Air

- Volume fractions less that $10^{-10}$ are show as white.
- At late time XSAGE has no cells with air volume fractions greater than a few percent. Without VOF this reduces to a fraction of a percent.



# Statement of the Obvious

- Clearly interface and thermal treatments can make significant differences, especially for late term mixing
- What to do?
  - Track interfaces
    - Easy in FronTier, perhaps not so easy for other codes
  - Reconstruct
    - E.g VOF
    - Still single temperature
- Enhance flow model to allow multiple temperatures

# Background: Equations of Motion

- Common methods for multi-temperature flow simulations:
  - Conserve component masses, total momentum, and total energy

$$\frac{\partial m_k r}{\partial t} + -\sum\left(m_k r \mathbf{u}\right) = 0$$

$$\frac{\partial r \mathbf{u}}{\partial t} + -\sum\left(r \mathbf{u} f \ \mathbf{u}\right) + -P = 0$$

$$\frac{\partial r\left(e + \frac{1}{2}u^2\right)}{\partial t} + -\sum r \mathbf{u}\left(e + \frac{1}{2}u^2\right) + -\sum P\mathbf{u} = 0$$

$r$ = total mass density, $m_k$ = mass fraction of component $k$, $\hat{\mathrm{A}}_{k=1}^{N} m_k = 1$

$\mathbf{u}$ = flow velocity, $P$ = pressure, $e$ = total specific internal energy

# Background: Equations of Motion – P-T Equilibrium

- The Euler system consists of *N+D +1* equations in *N+D+2* unknowns.
- Closure requires specifying a relation between the dependent variables
- Pressure-Temperature Equilibrium
  - Introduce micro-quantities
    - $V_k(P,T)$ : specific volume of component k
    - $e_k(P,T)$ : specific internal energy of component k
  - Closure Equations: $V = 1/r = \sum_{k=1}^{N} m_k V_k(P,T), e = \sum_{k=1}^{N} m_k e_k(P,T)$
  - Total system of *N+D+3* equations in *N+D+3* unknowns

# Background: P-T Equilibrium Microstructure

- **P-T equilibrium**: microstructure of the mixture consists of volumetrically distinct components in local mechanical (equal velocity and pressure) and thermal equilibrium.
  - Material components are separated by interfaces/contact discontinuities across which pressure and the interfacial normal component of velocity are continuous
  - Surface tension between components in the microstructure is negligible (no capillarity due to the microstructure)
  - Shear across the microstructure interface is negligible (common velocity)
  - The simulation time scales are sufficiently long that the components have time to come into thermal equilibrium due to un-modeled processes such as thermal conduction (common temperature)

# Background: Single Velocity/Single Pressure/Multiple Temperature Models

- Relax the condition of thermal equilibrium between material components by assuming each component in the microstructure has a separate temperature
- Missing *N-1* equations to close the system
- Constitutive equations are replaced by dynamic equations (PDE's)
- Two models are considered and implemented
  - Thermal Isolation:

$$T_k \frac{DS_k}{Dt} = \frac{De_k}{Dt} + P\frac{DV_k}{Dt} = 0, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}\sum\text{—}$$

  - Uniform Strain (more accurately uniform compression):

$$\frac{1}{V_k}\frac{DV_k}{Dt} = \frac{1}{V}\frac{DV}{Dt} = \text{—}\sum\mathbf{u}, \quad 1\,\text{£}\;\; k\,\text{£}\;\; N$$

# Background: Duality of the Models

- Models can be re-expressed as volume fraction equations:
  - $\alpha_k$ defined by $\alpha_k V = \mu_k V_k = \mu_k V_k(P, T_k)$
  - Thermal Isolation: $T_k \frac{DS_k}{Dt} = 0 \Rightarrow \frac{Da_k}{Dt} = a_k \left( \frac{\rho c^2}{\rho_k c_k^2} - 1 \right) \nabla \cdot \mathbf{u}, \quad \frac{1}{\rho c^2} = \sum_{k=1}^{N} \frac{a_k}{\rho_k c_k^2}$
  - Uniform Strain: $\frac{Da_k}{Dt} = 0 \Rightarrow T_k \frac{DS_k}{Dt} = \frac{c_k^2}{\Gamma_k} \left( 1 - \frac{\rho c^2}{\rho_k c_k^2} \right) \nabla \cdot \mathbf{u}, \rho c^2 = \frac{\sum_{k=1}^{N} \frac{a_k}{\Gamma_k} \rho_k c_k^2}{\sum_{k=1}^{N} \frac{a_k}{\Gamma_k}}.$
  - $c_k$ = component sound speed, $G_k$ = component Grüneisen exponent, and $c$ = mixture sound speed
  - Single sound speed model:

$$\frac{DP}{Dt} + \rho c^2 \nabla \cdot \mathbf{u} = 0$$

# Multi-Temperature Equation of State

- P-T equilibrium; compute pressure, temperature, and volume fractions given total specific volume, total specific internal energy, and mass fractions:

$$e = \sum_{k=1}^{N} m_k e_k\left(P,T\right),\ \ V = \sum_{k=1}^{N} m_k V_k\left(P,T\right) \text{ fi} \qquad \textbf{(PTE)}$$

$$P = P\left(e,V,m_1,\text{K},m_N\right), T = T\left(e,V,m_1,\text{K},m_N\right), a_k\left(e,V,m_1,\text{K},m_N\right) = \frac{m_k V_k\left(P,T\right)}{V}$$

- Thermal Isolation and Uniform strain: compute pressure given total specific volume, total specific internal energy, mass fractions, ***and*** volume fractions:

$$e = \sum_{k=1}^{N} m_k e_k\left(P,V_k\right),\ \ a_k V = m_1 V_k, T_k = T_k\left(P,V_k\right) \text{ fi} \qquad \textbf{(PE)}$$

$$P = P\left(e,V,m_1,\text{K},m_N,a_1,\text{K},a_N\right), T_k = T_k\left(e,V,m_1,\text{K},m_N,a_1,\text{K},a_N\right)$$

# Multiple Temperature Equation of State Observations

- The pressure equation is in the form to take advantage of single material component EOS.
- Most analytic equations of state in use for computational hydrodynamics are of the Grüneisen form:
  e.g.
  - Perfect (ideal) gases
  - Mie-Grüneisen
  - JWL

$$P - P_r(V) = \frac{\Gamma(V)}{V}\left(e - e_r(V)\right)$$

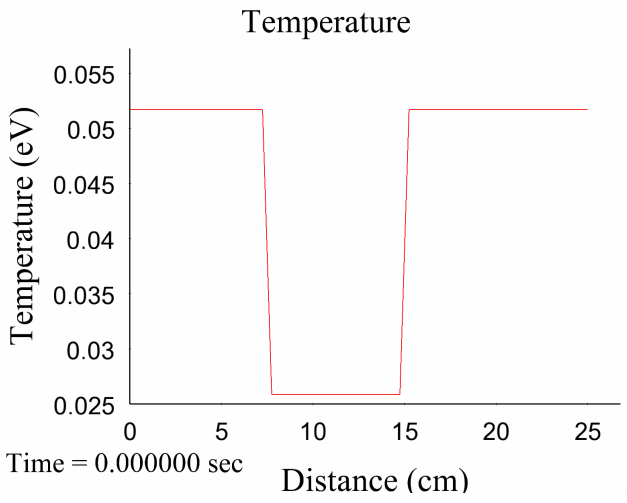
- If all of the component equations of state are of the Grüneisen form, then the mixture pressure equation is linear.
- Tabular equations of state can use a Newton method to compute the pressure
  - Numerical issues can occur due to poor interpolation
  - Bad sound speeds
  - Non-consistent thermodynamics (EOS not in free energy form)

# Test Problem: Hot Slab Translation

- Simple translation of a hot slab of material
  - Perfect gases with $\gamma_1 = \gamma_2 = 1.4$
  - Specific heats differ by a factor of 2, $C_{V,1} = 4.141 \times 10^{10}$ ergs/gram/eV , $C_{V,2} = 8.282 \times 10^{10}$ ergs/gram/eV
  - Constant density, pressure, specific internal energy, and velocity

$$\begin{pmatrix} \rho \\ P \\ e \\ u \end{pmatrix} = \begin{cases} 1.17 \times 10^{-3} \text{ grams/cc} \\ 10^{6} \ \mu\text{bar} \\ 1.49 \times 10^{9} \text{ ergs/gram} \\ 10^{6} \text{ cm/second} \end{cases}, 0 \leq x \leq 25 \text{ cm}$$

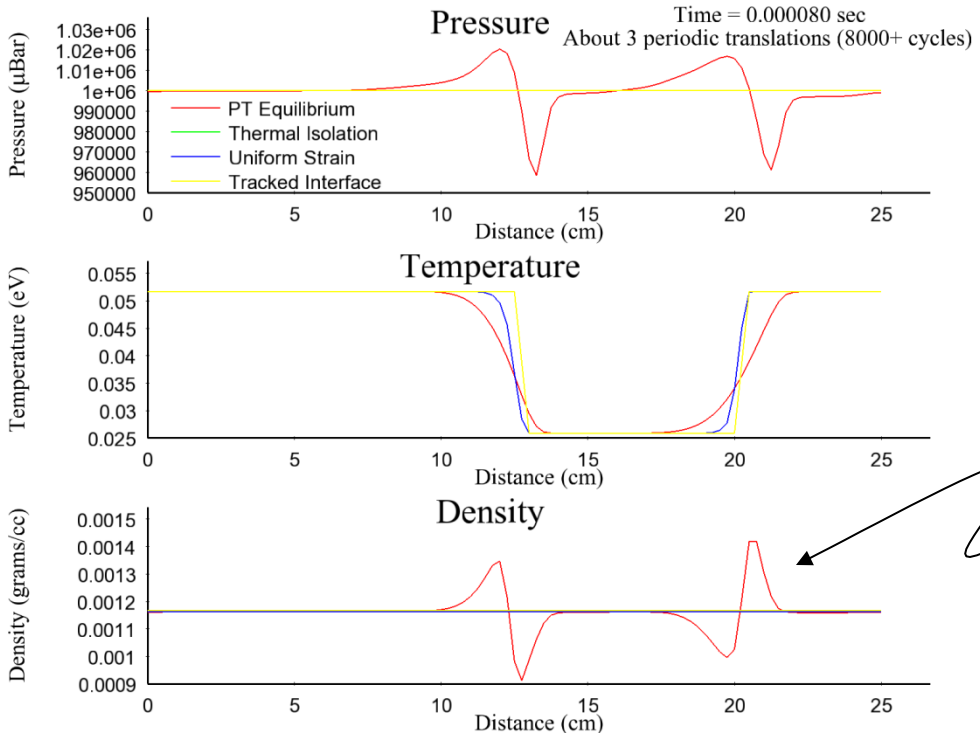
$$T = \begin{cases} 5.17 \times 10^{-2} \text{ eV}, \ 0 \leq x \leq 7.5, \ 15 \leq x \leq 25 \\ 2.59 \times 10^{-2} \text{ eV}, \ 7.5 \leq x \leq 15 \end{cases}$$



# Test Problem: Hot Slab Translation

- Solution shows that P-T equilibrium has a significant effect on the flow state

**≈ 8000 cycles**




**Transients created by the initial temperature discontinuity and then amplified by acoustic interactions.**

# Test Problem: Two Material Sod Problem

- Riemann problem with two material components
- Initial Conditions:
  - Two material components, both perfect gases
    - Component 1 initially in the interface $0 \le x \le 0.5$

      $\gamma_1 = 2.0$, $C_{V,1} = 10^{12}$ ergs/gram/eV
    - Component 2 initially in the interface $0.5 \le x \le 1$

      $\gamma_2 = 1.4$, $C_{V,2} = 10^{12}$ ergs/gram/eV
  - Isothermal initial conditions with a pressure/density jump across the interface

$$r\left(x,0\right) = \begin{cases} 10^{-3}\,\text{grams/cc} & 0 \le x \le 0.5\ \text{cm} \\ 1.25 \times 10^{-4}\,\text{grams/cc} & 0.5 \le x \le 1\ \text{cm} \end{cases}, \quad \text{P}(x,0) = \begin{cases} 2.0 \times 10^{6}\ \text{mbar} & 0 \le x \le 0.5\ \text{cm} \\ 10^{5}\ \text{mbar} & 0.5 \le x \le 1\ \text{cm} \end{cases}$$

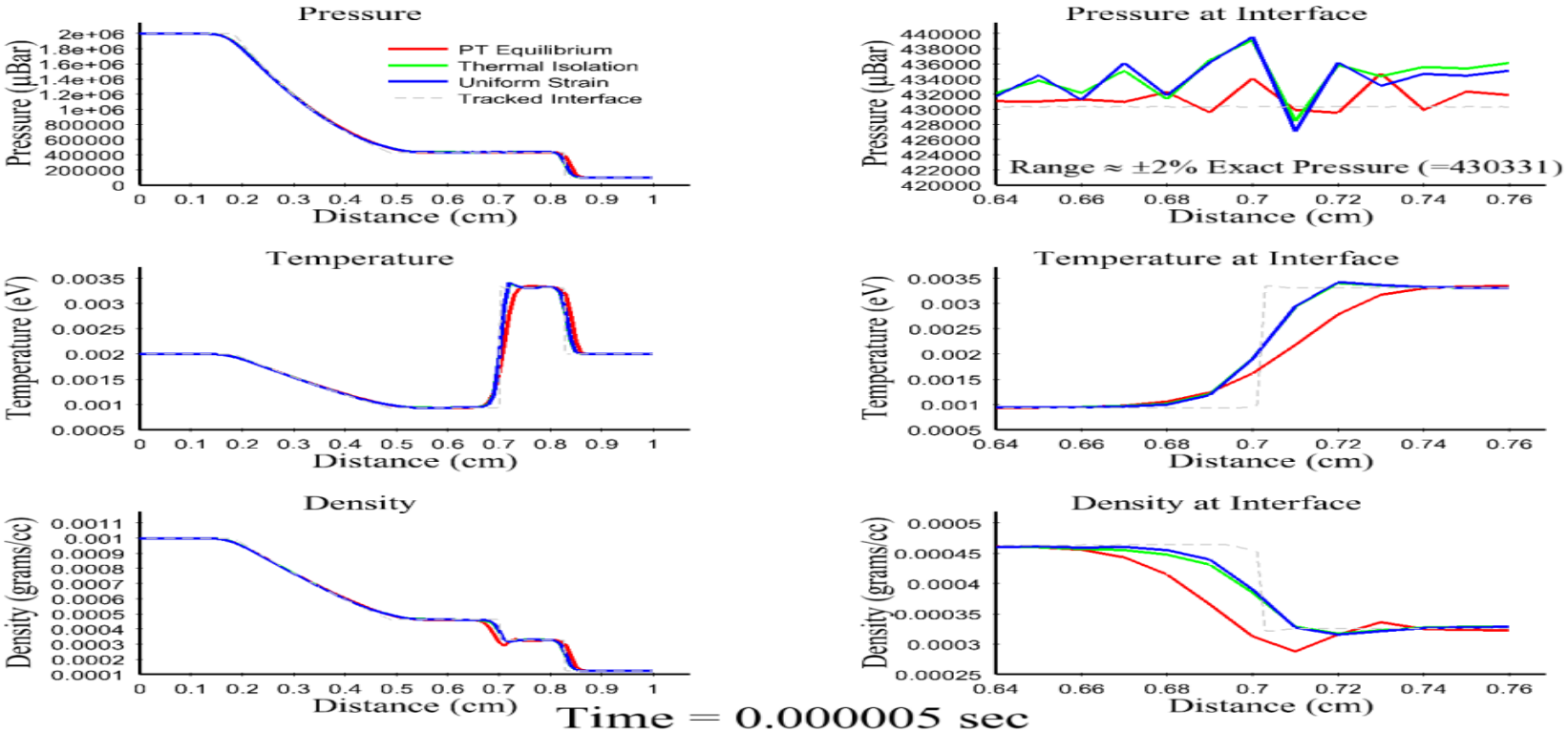
$$\text{u}(x,0) = 0 \quad | \quad 0 \le x \le 1\ \text{cm}$$

$$\text{e}(x,0) = 2.0 \times 10^{9}\ \text{ergs/gram} \quad | \quad 0 \le x \le 1\ \text{cm}, \quad \text{T}(x,0) = 2.0 \times 10^{-3}\ \text{eV} \quad | \quad 0 \le x \le 1\ \text{cm}$$

# Test Problem: Two Material Sod Problem

- Main effect to temperature equilibrium is an increase in the width of the transition layer at the interface

**1000 mesh zones**




Time = 0.000005 sec

**≈1000 cycles**

# Test Problem: Strong Shock Refraction

- A Mach 15 shock accelerates the interface between two materials
- Initial Conditions:
  - Spherical Symmetry
  - Two material components, both perfect gases
    - Component 1 initially in the interface $0 \le x \le 3$ cm

      $\gamma_1 = 1.1$, $C_{V,1} = 4\times10^{10}$ ergs/gram/eV
    - Component 2 initially in the interface $3 \le x \le 10$ cm

      $\gamma_2 = 2.0$, $C_{V,2} = 4\times10^{6}$ ergs/gram/eV
  - Isothermal initial conditions with a density jump across the interface

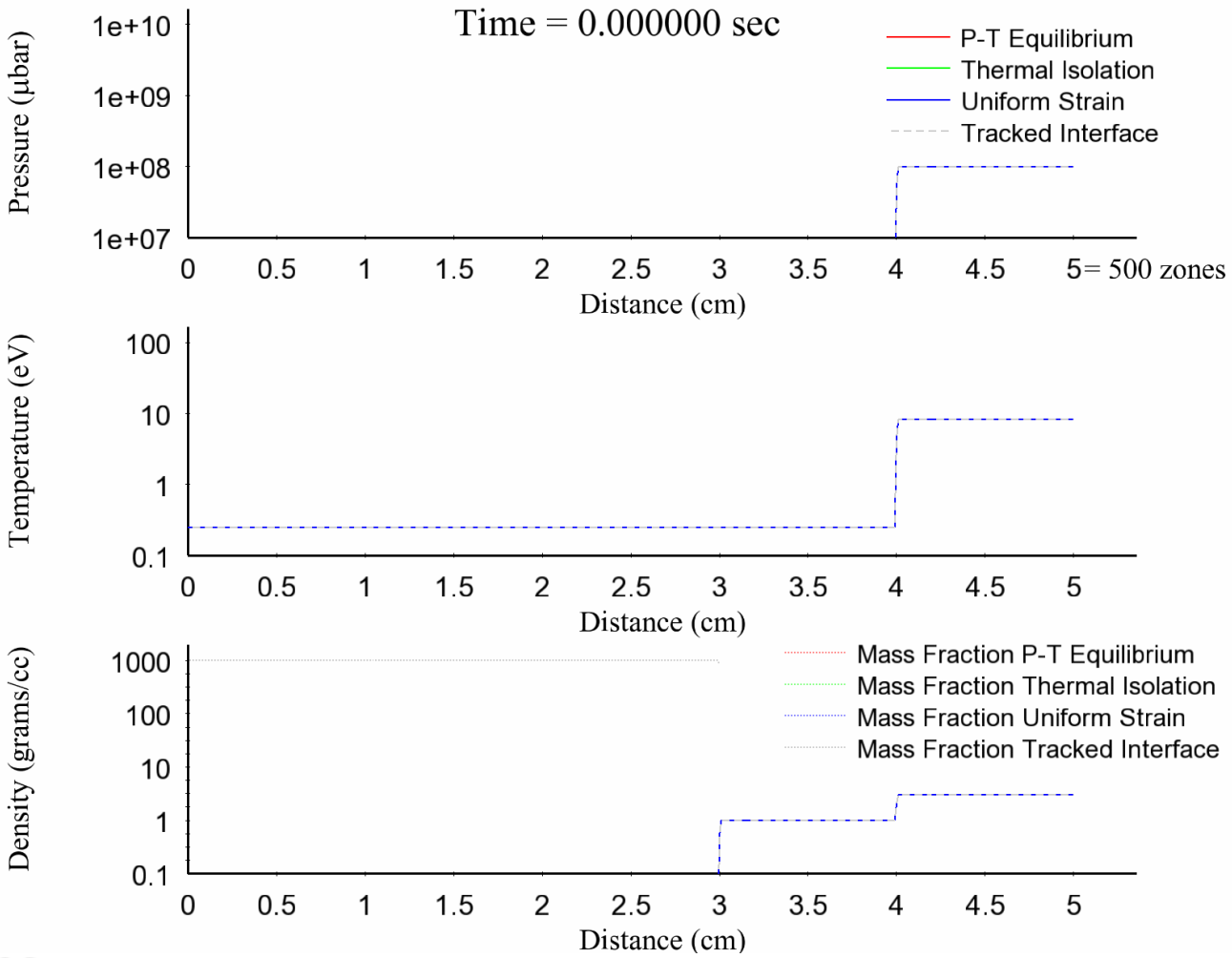
$$r(x,0) = \begin{cases} 10^{-3}\ \text{grams/cc} & 0 \le x \le 3\ \text{cm} \\ 1.0\ \text{grams/cc} & 3 \le x \le 4\ \text{cm} \end{cases}, \quad e(x,0) = \begin{cases} 10^{10}\ \text{ergs/gram} & 0 \le x \le 3\ \text{cm} \\ 10^{6}\ \text{ergs/gram} & 3 \le x \le 4\ \text{cm} \end{cases}$$

$$\text{P(x,0)}=10^{6}\ \mu\text{bar} \mid 0 \le x \le 4\ \text{cm}$$

$$\text{u(x,0)}=0 \mid 0 \le x \le 4\ \text{cm},\ \text{T(x,0)}=0.25\ \text{eV} \mid 0 \le x \le 3\ \text{cm}$$

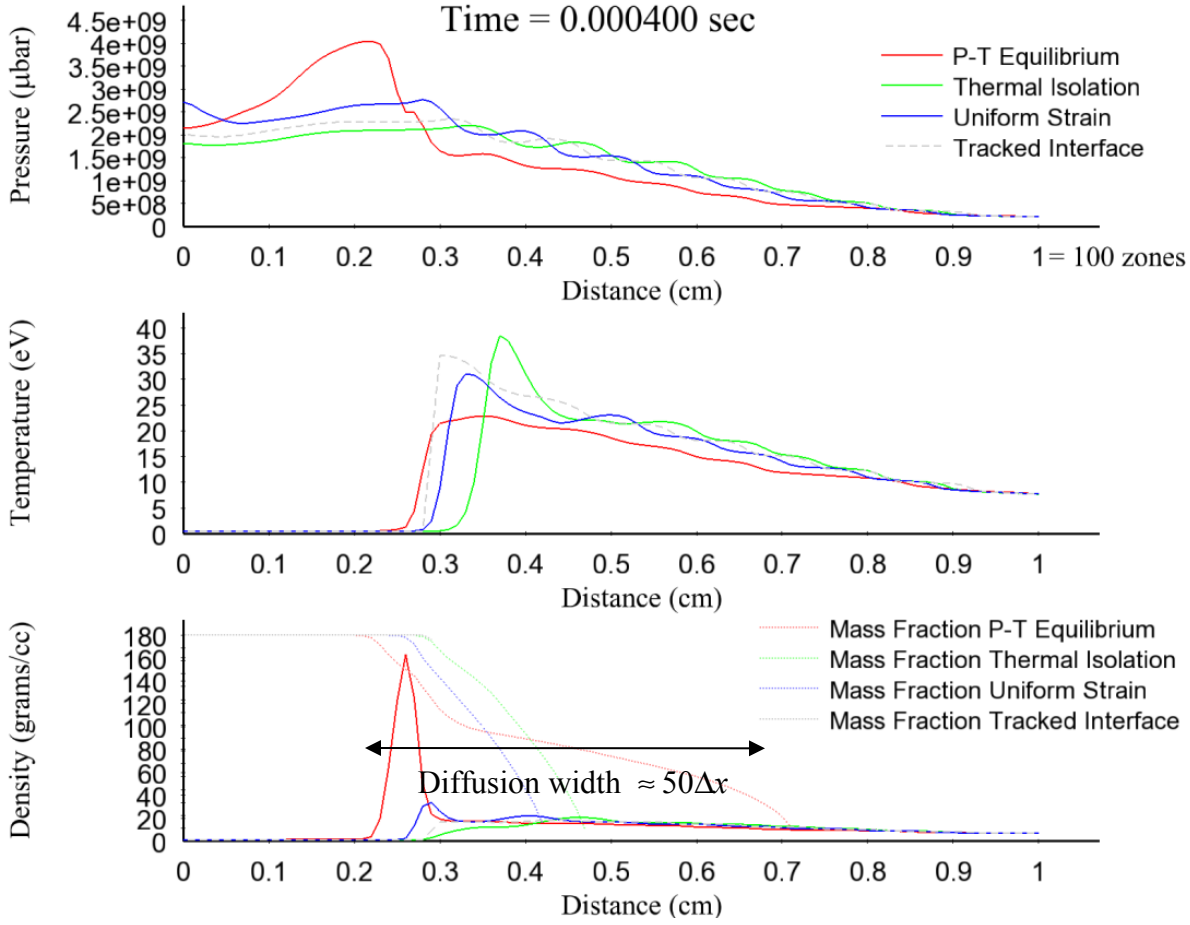
  - A density of 3 grams/cc and a pressure of $10^8$ μbar is initialized for the region $4 \le x \le 10$ cm , with zero initial velocity

# Test Problem: Strong Shock Refraction



# Test Problem: Strong Shock Refraction

- P-T equilibrium has fast wave speed and much broader diffusion layer



# Issues, Shock Structure

- The thermal isolation and the uniform strain model are not in first principles conservation form
  - The "total" Hugoniot $e - e_0 = 0.5(P+P_0)(V_0 - V)$ is under-determined
  - Conservation of mass implies mass fractions are constant across shocks
  - For thermal isolation, a natural shock assumption is the separate Hugoniot solution:
    - Each component shocks to a common pressure using its separate Hugoniot equation
    - Solution to the mixture total specific internal energy, pressure, total specific volume Hugoniot
    - Ensures a $C^2$ combined rarefaction/Hugoniot wave curve
  - For uniform strain the natural assumption is that volume fractions are constant across shocks
    - Consistent with the advection assumption for volume fractions
    - Provides sufficient information to solve the "total" Hugoniot equation
    - Ensures a $C^2$ combined rarefaction/Hugoniot wave curve
- In both cases the effective shock Hugoniot is determined by the numerical viscosity of the finite difference scheme

# Conclusions/Observations

- Ideally, for inviscid flows and immiscible flows FronTier style interface tracking is an ideal and nature approach
  - Not very easy to retrofit into existing codes
  - Framework in fact also supports miscible flows
    - Without tracking
    - With tracking – leaky interfaces
- Multi-Temperature flows can substantially reduce thermal and mixing layers
  - Issues with “poor” EOS’s (tabular)
- Multiple-pressure schemes are promising but introduce additional modeling concerns
  - E.g. velocity non-equilibrium
  - Relaxation equations are generally numerical.